10/049, 164

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NEWS EXPRESS JUNE 13 CURRENT WINDOWS VERSION IS V8.0, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0jc(JP), AND CURRENT DISCOVER FILE IS DATED 13 JUNE 2005

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FILE 'HOME' ENTERED AT 15:31:37 ON 19 SEP 2005

=> FIL REGISTRY COST IN U.S. DOLLARS

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* effective March 20, 2005. A new display format, IDERL, is now

* available and contains the CA role and document type information.

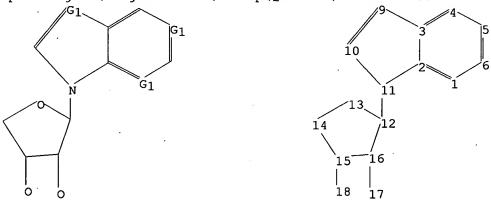
*

Structure search iteration limits have been increased. See HELP SLIMITS for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

=>

Uploading C:\Program Files\Stnexp\Queries\10049164.str



chain nodes : 17 18 ring nodes : 1 2 3 4 5 10 11 12 13 14 69 chain bonds : 11-12 15-18 16-17 ring bonds : 1-2 1-6 2-3 2-11 3-4 3-9 4-5 5-6 9-10 10-11 12-13 12-16 13-14 14-15 15-16 exact/norm bonds : 1-2 1-6 2-3 2-11 3-4 3-9 4-5 5-6 9-10 10-11 11-12 12-13 12-16 13-14 14-15 15-16 15-18 16-17 isolated ring systems : containing 1 : 12 :

G1:C,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS 18:CLASS

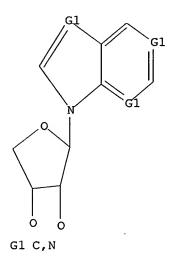
STRUCTURE UPLOADED L1

=> d 11

L1 HAS NO ANSWERS

L1

STR



Structure attributes must be viewed using STN Express query preparation.

=> s 11

SAMPLE SEARCH INITIATED 15:32:08 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 3216 TO ITERATE

62.2% PROCESSED 2000 ITERATIONS 50 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 60919 TO 67721

PROJECTED ANSWERS: 54755 TO 61213

50 SEA SSS SAM L1 L2

=> s ll sss full

FULL SEARCH INITIATED 15:32:16 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 65169 TO ITERATE

65169 ITERATIONS 100.0% PROCESSED 58171 ANSWERS

SEARCH TIME: 00.00.01

L3 58171 SEA SSS FUL L1

=> FIL CAPLUS

COST IN U.S. DOLLARS SINCE FILE TOTAL

ENTRY SESSION

FULL ESTIMATED COST 161.33 161.54

FILE 'CAPLUS' ENTERED AT 15:32:23 ON 19 SEP 2005 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2005 AMERICAN CHEMICAL SOCIETY (ACS)

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FILE COVERS 1907 - 19 Sep 2005 VOL 143 ISS 13 FILE LAST UPDATED: 18 Sep 2005 (20050918/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 13

207164 L3

=> s 14 and fluorescen? probe

405555 FLUORESCEN?

213499 PROBE

107218 PROBES

283011 PROBE

(PROBE OR PROBES)

12819 FLUORESCEN? PROBE

(FLUORESCEN? (W) PROBE)

L5 484 L4 AND FLUORESCEN? PROBE

=> s 15 and activity(W)based

2058993 ACTIVITY

404479 ACTIVITIES

2226737 ACTIVITY

(ACTIVITY OR ACTIVITIES)

1798409 BASED

1648 ACTIVITY (W) BASED

L6 2 L5 AND ACTIVITY (W) BASED

=> d 16 ibib abs hitstr tot

ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

2002:899767 CAPLUS

DOCUMENT NUMBER:

138:250529

TITLE:

Trifunctional chemical probes for the consolidated

detection and identification of enzyme activities from

complex proteomes

AUTHOR(S):

Adam, Gregory C.; Sorensen, Erik J.; Cravatt, Benjamin

CORPORATE SOURCE:

The Skaggs Institute for Chemical Biology and the

Department of Chemistry, The Scripps Research Institute, La Jolla, CA, 92037, USA

SOURCE:

Molecular and Cellular Proteomics (2002), 1(10),

828-835

CODEN: MCPOBS; ISSN: 1535-9476

PUBLISHER:

American Society for Biochemistry and Molecular

Biology, Inc.

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 138:250529

Chemical probes that covalently modify the active sites of enzymes in complex AB proteomes are useful tools for identifying enzyme activities associated with discrete (patho)physiol. states. Researchers in proteomics typically use two types of activity-based probes to fulfill complementary objectives: fluorescent probes for rapid and sensitive target detection and biotinylated probes for target purification and identification. Accordingly, we hypothesized that a strategy in which the target detection and target isolation steps of activitybased proteomic expts. were merged might accelerate the characterization of differentially expressed protein activities. report the synthesis and application of trifunctional chemical proteomic probes in which elements for both target detection (e.g. rhodamine) and isolation (e.g. biotin) are appended to a sulfonate ester reactive group, permitting the consolidated visualization and affinity purification of labeled proteins by a combination of in-gel fluorescence and avidin chromatog. procedures. A trifunctional Ph sulfonate probe was used to identify several tech. challenging protein targets, including the integral membrane enzyme 3β -hydroxysteroid dehydrogenase/ Δ 5-isomerase and the cofactor-dependent enzymes platelet-type phosphofructokinase and type II tissue transglutaminase. The latter two enzyme activities were significantly up-regulated in the invasive estrogen receptor-neq. (ER(-)) human breast cancer cell line MDA-MB-231 relative to the non-invasive ER(+) breast cancer lines MCF7 and T-47D. Collectively these studies demonstrate that chemical proteomic probes incorporating elements for both target detection and target isolation fortify the important link between the visualization of differentially expressed enzyme activities and their subsequent mol. identification, thereby augmenting the information content achieved in activity-based profiling expts.

IT 56-65-5, 5'-ATP, biological studies

RL: BSU (Biological study, unclassified); BIOL (Biological study) (labeling of platelet-type phosphofructokinase by trifunctional Ph sulfonate probe is inhibited by ATP)

RN 56-65-5 CAPLUS

CN Adenosine 5'-(tetrahydrogen triphosphate) (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:615942 CAPLUS

DOCUMENT NUMBER: 137:165832

TITLE: Activity based probe analysis

INVENTOR(S):
Patricelli, Matthew P.

PATENT ASSIGNEE(S): Activx Biosciences, Inc., USA

SOURCE: PCT Int. Appl., 62 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent English

LANGUAGE:

Engli

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PA!	KIND DATE				APPLICATION NO.						DATE							
	WO 2002063271														20020205			
						C1 20021024												
WO	2002	A3 200307			0710													
	W:	ΑE,	AG,	AL,	AM,	AT,	AU,	ΑZ,	BA,	BB,	BG,	BR,	BY,	BZ,	CA,	CH,	CN,	
							DK,											
		GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KP,	KR,	KZ,	LC,	LK,	LR,	
		LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NO,	NZ,	OM,	PH,	
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-		KG,	ΚZ,	MD,	RU,	ТJ,	TM,	AT,	BE,	CH,	CY,	DE,	DK,	ES,	FI,	FR,	GB,	
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EP	EP 1364209						A2 20031126			EP 2	002-	7148	20020205					
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US	US 2003175986					A1 20030918			US 2002-49164					20021021				
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					•			1	US 2	001-	33942	1	P 20011211					
									1	WO 2	002-1	US380	80	1	√ 2	0020	205	
OTHER SO		MARPAT 137:165832																

OTHER SOURCE(S): MARPAT 137:165832

AB The invention concerns methods and compns. are described for analyzing complex protein mixts. using fluorescent activity-based probes. In particular, probes that specifically react with and bind to the active form of one or more target proteins are employed. Fluorescent signals obtained from the labeled active target proteins can be related to the presence or amount of active members of the desired target protein class. The methods and compns. described herein can be used, for example, to provide diagnostic information concerning pathogenic states, in identifying proteins that may act as therapeutic targets, and in drug discovery.

IT 446850-50-6P 446850-53-9P 446850-55-1DP,
reaction with rhodamine green 446850-58-4P 446850-61-9P
446850-64-2P 446850-67-5P 446850-69-7DP,
reaction with rhodamine green 446850-71-1P 446850-73-3P
446850-76-6P 446850-79-9P 446850-81-3P
RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST

RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST
(Analytical study); PREP (Preparation); USES (Uses)
 (activity based probe anal.)

RN. 446850-50-6 CAPLUS

CN Adenosine, 5'-deoxy-5'-[[(1,1-dimethylethoxy)carbonyl]amino]-, 2'(or 3')-[(2-aminoethyl)carbamate] (9CI) (CA INDEX NAME)

CM 1

CRN 446850-49-3 CMF C15 H22 N6 O5

CRN 109-58-0 CMF C3 H8 N2 O2

 $H_2N-CH_2-CH_2-NH-CO_2H$

RN 446850-53-9 CAPLUS

CN Adenosine, 5'-amino-5'-deoxy-, monoester with 9-[2-carboxy-4(or 5)-[[[2-(carboxyamino)ethyl]amino]carbonyl]phenyl]-3,6-bis(dimethylamino)xanthylium inner salt (9CI) (CA INDEX NAME)

CM 1

CRN 446850-52-8 CMF C28 H28 N4 O6

CCI IDS

CM 2

CRN 14365-44-7 CMF C10 H14 N6 O3

RN 446850-55-1 CAPLUS

CN Adenosine, 5'-amino-5'-deoxy-, 2'(or 3')-[(2-aminoethyl)carbamate] (9CI) (CA INDEX NAME)

CM 1

CRN 14365-44-7 CMF C10 H14 N6 O3

Absolute stereochemistry.

CM 2

CRN 109-58-0 CMF C3 H8 N2 O2

 $H_2N-CH_2-CH_2-NH-CO_2H$

RN 446850-58-4 CAPLUS

CN Adenosine, 5'-deoxy-5'-[[4-(fluorosulfonyl)benzoyl]amino]-, 2'(or 3')-[[2-[[3(or 4)-[3,6-bis(dimethylamino)xanthylium-9-yl]-4(or 3)-carboxybenzoyl]amino]ethyl]carbamate], inner salt (9CI) (CA INDEX NAME)

CM 1

CRN 446850-57-3 CMF C17 H17 F N6 O6 S

CRN 446850-52-8 CMF C28 H28 N4 O6 CCI IDS

RN 446850-61-9 CAPLUS

CN Adenosine, 5'-deoxy-5'-[[4-(ethenylsulfonyl)benzoyl]amino]-, 2'(or 3')-[[2-[[3(or 4)-[3,6-bis(dimethylamino)xanthylium-9-yl]-4(or 3)-carboxybenzoyl]amino]ethyl]carbamate], inner salt (9CI) (CA INDEX NAME)

CM 1

CRN 446850-60-8 CMF C19 H20 N6 O6 S

CRN 446850-52-8 CMF C28 H28 N4 O6 CCI IDS

RN 446850-64-2 CAPLUS

CN Adenosine, 5'-deoxy-5'-[(1-oxo-2-propenyl)amino]-, 2'(or 3')-[[2-[[3(or 4)-[3,6-bis(dimethylamino)xanthylium-9-yl]-4(or 3)-carboxybenzoyl]amino]ethyl]carbamate], inner salt (9CI) (CA INDEX NAME)

CM 1

CRN 446850-63-1 CMF C13 H16 N6 O4

CRN 446850-52-8 C28 H28 N4 O6 CMF

CCI IDS

RN 446850-67-5 CAPLUS

CN Adenosine, 5'-[(2-chloro-1-oxo-2-propenyl)amino]-5'-deoxy-, 2'(or 3')-[[2-[[3(or 4)-[3,6-bis(dimethylamino)xanthylium-9-yl]-4(or 3)-carboxybenzoyl]amino]ethyl]carbamate], inner salt (9CI) (CA INDEX NAME)

CM 1

446850-66-4 CRN CMF C13 H15 C1 N6 O4

Absolute stereochemistry.

2 CM

CRN 446850-52-8 C28 H28 N4 O6 CMF

CCI IDS

RN 446850-69-7 CAPLUS

CN Adenosine, 5'-deoxy-5'-[[4-(fluorosulfonyl)benzoyl]amino]-, 2'(or 3')-[(2-aminoethyl)carbamate] (9CI) (CA INDEX NAME)

CM 1

CRN 446850-57-3

CMF C17 H17 F N6 O6 S

Absolute stereochemistry.

CM 2

CRN 109-58-0

CMF C3 H8 N2 O2

 $H_2N-CH_2-CH_2-NH-CO_2H$

RN 446850-71-1 CAPLUS

CN Adenosine, 5'-O-[(4-methoxyphenyl)diphenylmethyl]-, 2'(or 3')-[(2-aminoethyl)carbamate] (9CI) (CA INDEX NAME)

CM 1

CRN 51600-11-4

CMF C30 H29 N5 O5

CRN 109-58-0 CMF C3 H8 N2 O2

H2N-СH2-СH2-NH-СО2Н

RN 446850-73-3 CAPLUS

CN Adenosine, 2'(or 3')-[[2-[[3(or 4)-[3,6-bis(dimethylamino)xanthylium-9-yl]-4(or 3)-carboxybenzoyl]amino]ethyl]carbamate], inner salt (9CI) (CA INDEX NAME)

CM 1

CRN 446850-52-8 CMF C28 H28 N4 O6 CCI IDS

CM 2

CRN 58-61-7 CMF C10 H13 N5 O4

RN 446850-76-6 CAPLUS

CN Adenosine, 2'(or 3')-[[2-[[3(or 4)-[3,6-bis(dimethylamino)xanthylium-9-yl]-4(or 3)-carboxybenzoyl]amino]ethyl]carbamate] 5'-(chloroacetate), inner salt (9CI) (CA INDEX NAME)

CM 1

CRN 446850-75-5 CMF C12 H14 C1 N5 O5

Absolute stereochemistry.

CM 2

CRN 446850-52-8 CMF C28 H28 N4 O6 CCI IDS

RN 446850-79-9 CAPLUS

CN Adenosine, $2'(\text{or }3')-[[2-[[3(\text{or }4)-[3,6-\text{bis}(\text{dimethylamino})\,xanthylium-9-yl]}-$

4(or 3)-carboxybenzoyl]amino]ethyl]carbamate] 5'-[4-(fluorosulfonyl)benzoate], inner salt (9CI) (CA INDEX NAME)

CM 1

CRN 446850-52-8 CMF C28 H28 N4 O6

CCI IDS

CM 2

CRN 57454-44-1 CMF C17 H16 F N5 O7 S

Absolute stereochemistry.

RN 446850-81-3 CAPLUS

CN Adenosine, 5'-amino-5'-deoxy-, 2'(or 3')-[[2-[[3(or 4)-[3,6-bis(dimethylamino)xanthylium-9-yl]-4(or 3)-carboxybenzoyl]amino]ethyl]carb amate], inner salt, trifluoroacetate (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 76-05-1 CMF C2 H F3 O2

CRN 446850-53-9 CMF C38 H40 N10 O8

CCI IDS

CM 3

CRN 446850-52-8 CMF C28 H28 N4 O6 CCI IDS

CM 4

CRN 14365-44-7 CMF C10 H14 N6 O3

Absolute stereochemistry.

=> s 15 and tag 20980 TAG 8077 TAGS => 17 not 16

L7 IS NOT A RECOGNIZED COMMAND

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=> s 17 not 16

L8 2 L7 NOT L6

=> dup rem 16 17

PUBLISHER:

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9 4 DUP REM L6 L7 (0 DUPLICATES REMOVED)
ANSWERS '1-4' FROM FILE CAPLUS

=> d 17 ibib abs hitstr tot

L7 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2003:871776 CAPLUS

DOCUMENT NUMBER: 141:49860

TITLE: Molecular Properties of Purified Human Uncoupling

Protein 2 Refolded from Bacterial Inclusion Bodies

AUTHOR(S): Jekabsons, Mika B.; Echtay, Karim S.; Arechaga,

Ignacio; Brand, Martin D.

CORPORATE SOURCE: Dunn Human Nutrition Unit, Medical Research Council,

Cambridge, CB2 2XY, UK

SOURCE: Journal of Bioenergetics and Biomembranes (2003),

35(5), 409-418

CODEN: JBBID4; ISSN: 0145-479X Kluwer Academic/Plenum Publishers

DOCUMENT TYPE: Journal LANGUAGE: English

One way to study low-abundance mammalian mitochondrial carriers is by ectopically expressing them as bacterial inclusion bodies. Problems encountered with this approach include protein refolding, homogeneity, and stability. In this study, we investigated protein refolding and homogeneity properties of inclusion body human uncoupling protein 2 (UCP2). N-methylanthraniloyl-tagged ATP (Mant-ATP) expts. indicated two independent inclusion body UCP2 binding sites with dissociation consts. (Kd) of 0.3-0.5 and 23-92 μM . Dimethylanthranilate, the fluorescent tag without nucleotide, bound with a Kd of greater than 100 μM, suggesting that the low affinity site reflected binding of the tag By direct titration, UCP2 bound [8-14C] ATP and [8-14C] ADP with Kds of 4-5 and 16-18 μM , resp. Mg2+ (2 mM) reduced the apparent ATP affinity to 53 µM, an effect entirely explained by chelation of ATP; with Mq2+, Kd using calculated free ATP was 3 μM. A combination of gel filtration, Cu2+-phenanthroline crosslinking, and ultracentrifugation indicated that 75-80% of UCP2 was in a monodisperse, 197 kDa form while the remainder was aggregated. We conclude that (a) Mant-tagged nucleotides are useful fluorescent probes with isolated UCP2 when used with dimethylanthranilate controls; (b) UCP2 binds Mg2+-free nucleotides: the Kd for ATP is about 3-5 µM and for Mant-ATP it is about 10 times lower; and (c) in C12E9 detergent, the monodisperse protein may be in dimeric form.

IT 56-65-5, 5'-ATP, biological studies 58-64-0, 5'-ADP, biological studies

RL: BSU (Biological study, unclassified); BIOL (Biological study) (FRET fluorescence of N-methylanthraniloyl-tagged ATP as method of assessing nucleotide binding to purified human uncoupling protein 2

using dimethylanthranilate controls)

RN 56-65-5 CAPLUS

CN Adenosine 5'-(tetrahydrogen triphosphate) (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 58-64-0 CAPLUS

CN Adenosine 5'-(trihydrogen diphosphate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 85287-56-5

RL: BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)

(FRET fluorescence of N-methylanthraniloyl-tagged ATP as method of assessing nucleotide binding to purified human uncoupling protein 2 using dimethylanthranilate controls)

RN 85287-56-5 CAPLUS

CN Adenosine 5'-(tetrahydrogen triphosphate), 3'-[2-(methylamino)benzoate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.

32

REFERENCE COUNT:

THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 2 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN

2002:90063 CAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 136:163716

TITLE: Labeled peptides, proteins and antibodies and

processes and intermediates useful for their

preparation

INVENTOR(S): Hahn, Klaus M.; Toutchkine, Alexei; Muthyala, Rajeev;

Kraynov, Vadim; Bark, Steven J.; Burton, Dennis R.;

Chamberlain, Chester

The Scripps Research Institute, USA PATENT ASSIGNEE(S):

SOURCE: PCT Int. Appl., 158 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PA	PATENT NO.						KIND DATE			APPLICATION NO.						DATE			
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	W:	ΑE,	AG,	AL,	AM,	ΑT,	AU,	ΑZ,	BA,	BB,	BG,	BR,	BY,	BZ,	CA,	CH,	CN,		
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									1	WO 2	001-1	US22	194	1	v 2	0010	713		
HER S	OURCE		MARPAT 136:163716																

The invention provides peptide synthons having protected functional groups for attachment of desired moieties (e.g. functional mols. or probes). Also provided are peptide conjugates prepared from such synthons, and synthon and conjugate preparation methods including procedures for identifying optimum probe attachment sites. Biosensors are provided having functional mols. that can locate and bind to specific biomols. within living cells. Biosensors can detect chemical and physiol. changes in those biomols. as living cells are moving, metabolizing and reacting to its environment. Methods are included for detecting GTP activation of a Rho GTPase protein using polypeptide biosensors. When the biosensor binds GTP-activated Rho

GTPase protein, an environmentally sensitive dye emits a signal of a different lifetime, intensity or wavelength than when not bound. New fluorophores whose fluorescence responds to environmental changes are also provided that have improved detection and attachment properties, and that can be used in living cells, or in vitro.

IT 56-65-5, ATP, biological studies 86-01-1, GTP
RL: BSU (Biological study, unclassified); BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)

(labeled peptides, proteins and antibodies and processes and intermediates useful for preparation)

RN 56-65-5 CAPLUS

CN Adenosine 5'-(tetrahydrogen triphosphate) (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 86-01-1 CAPLUS

CN Guanosine 5'-(tetrahydrogen triphosphate) (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.

=> s 14 and tag

20980 TAG

8077 TAGS

24726 TAG

(TAG OR TAGS)

L10 372 L4 AND TAG

=> 110 and protein

L10 IS NOT A RECOGNIZED COMMAND

The previous command name entered was not recognized by the system. For a list of commands available to you in the current file, enter "HELP COMMANDS" at an arrow prompt (=>).

=> s 110 and protein

1785091 PROTEIN

1243217 PROTEINS

2074982 PROTEIN

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(PROTEIN OR PROTEINS)
L11
           304 L10 AND PROTEIN
=> s 111 and conjugate
         61979 CONJUGATE
         54913 CONJUGATES
        95734 CONJUGATE
                 (CONJUGATE OR CONJUGATES)
           27 L11 AND CONJUGATE
L12
=> s 112 and label
        58073 LABEL
        19704 LABELS
         69584 LABEL
                 (LABEL OR LABELS)
L13
            4 L12 AND LABEL
=> s 113 not 19
            2 S L9
L15
            2 S L9
L16
            4 L13 NOT (L14 OR L15)
=> d 113 ibib abs hitstr tot
L13 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2005 ACS on STN
                        2004:1037349 CAPLUS
ACCESSION NUMBER:
DOCUMENT NUMBER:
                        142:19000
TITLE:
                        Labeling of fusion proteins by enzymic
                        incorporation of a coenzyme A derivative into an acyl
                        carrier protein moiety
                        Johnsson, Kai; George, Nathalie
INVENTOR(S):
PATENT ASSIGNEE(S):
                        EPFL-Ecole Polytechnique Federale de Lausanne, Switz.
                        PCT Int. Appl., 46 pp.
SOURCE:
                        CODEN: PIXXD2
DOCUMENT TYPE:
                        Patent
LANGUAGE:
                        English
FAMILY ACC. NUM. COUNT:
PATENT INFORMATION:
    PATENT NO.
                        KIND
                               DATE
                                           APPLICATION NO.
                                                                DATE
                               -----
                        ____
                                           ______
                                                                 _____
    WO 2004104588
                        A1
                               20041202
                                         WO 2004-IB1733
                                                                  20040519
        W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
            CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
            GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
            LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
            NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
            TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
        RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
            AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
            EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE,
            SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GO, GW, ML, MR, NE,
            SN, TD, TG
PRIORITY APPLN. INFO.:
                                           EP 2003-405364 A 20030523
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PRIORITY APPLN. INFO.:

OTHER SOURCE(S):

MARPAT 142:19000

AB A method for labeling acyl carrier protein (ACP) fusion

proteins using derivs. of CoA is described. The method relies on
the transfer of a label from a CoA type substrate to an ACP
fusion protein using a holo-acyl carrier protein
synthase (ACPS) or a homolog thereof. The method allows detecting and
manipulating the fusion protein, both in vitro and in vivo, by
attaching mols. to the fusion proteins that introduce a new
phys. or chemical property to the fusion protein. Examples of such

labels are, among others, spectroscopic probes or reporter mols., affinity tags, mols. generating reactive radicals, cross-linkers, ligands mediating protein-protein interactions or mols. suitable for the immobilization of the fusion protein. Synthesis of a series of reporter mol. conjugates, including digoxigenin, Cy3 and Cy5, with CoA is reported.

IT 85-61-0D, Coenzyme A, derivs.

RL: BUU (Biological use, unclassified); RCT (Reactant); BIOL (Biological study); RACT (Reactant or reagent); USES (Uses)

(labeling of acyl carrier **protein** with; labeling of fusion **proteins** by enzymic incorporation of coenzyme derivative into acyl carrier **protein** moiety)

RN 85-61-0 CAPLUS

CN Coenzyme A (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

PAGE 1-B

TT 756898-07-4P 756898-08-5P 756898-09-6P 756898-10-9P

RL: ARU (Analytical role, unclassified); BUU (Biological use, unclassified); SPN (Synthetic preparation); ANST (Analytical study); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation and labeling use of; labeling of fusion **proteins** by enzymic incorporation of coenzyme derivative into acyl carrier **protein** moiety)

RN 756898-07-4 CAPLUS

CN Coenzyme A, S-[1-[6-[2-[5-[(3aS,4S,6aR)-hexahydro-2-oxo-1H-thieno[3,4-d]imidazol-4-yl]-1-oxopentyl]hydrazino]-6-oxohexyl]-2,5-dioxo-3-pyrrolidinyl]- (9CI) (CA INDEX NAME)

PAGE 1-B

RN 756898-08-5 CAPLUS
CN Coenzyme A, S-[1-[6-[2-[4-[[(3β,5β,12β,14β)-21,23-epoxy-12,14-dihydroxy-23-oxo-24-norchol-20(22)-en-3-yl]amino]-1,4-dioxobutyl]hydrazino]-6-oxohexyl]-2,5-dioxo-3-pyrrolidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

PAGE 1-C

RN 756898-09-6 CAPLUS

CN Coenzyme A, S-[1-[2-[[6-[2-[3-(1-ethyl-1,3-dihydro-3,3-dimethyl-5-sulfo-2H-indol-2-ylidene)-1-propenyl]-3,3-dimethyl-5-sulfo-3H-indolio]-1-oxohexyl]amino]ethyl]-2,5-dioxo-3-pyrrolidinyl]-, inner salt (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry unknown.

PAGE 1-B

RN 756898-10-9 CAPLUS

CN Coenzyme A, S-[1-[2-[[6-[2-[5-(1-ethyl-1,3-dihydro-3,3-dimethyl-5-sulfo-2H-indol-2-ylidene)-1,3-pentadienyl]-3,3-dimethyl-5-sulfo-3H-indolio]-1-oxohexyl]amino]ethyl]-2,5-dioxo-3-pyrrolidinyl]-, inner salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

PAGE 1-B

REFERENCE COUNT:

THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

2004:350520 CAPLUS

DOCUMENT NUMBER:

141:119215

TITLE:

Elucidation of eukaryotic elongation factor-2 contact

sites within the catalytic domain of Pseudomonas

aeruginosa exotoxin A

AUTHOR(S):

Yates, Susan P.; Merrill, Allan R.

CORPORATE SOURCE:

Guelph-Waterloo Centre for Graduate Work in Chemistry

and Biochemistry, Department of Chemistry and

Biochemistry, University of Guelph, Guelph, ON, N1G

2W1, Can.

SOURCE:

Biochemical Journal (2004), 379(3), 563-572

CODEN: BIJOAK; ISSN: 0264-6021

PUBLISHER:

Portland Press Ltd.

DOCUMENT TYPE:

Journal English

LANGUAGE:

3 Pseudomonas aeruginosa produces the virulence factor, ETA (exotoxin A),

which catalyzes an ADP-ribosyltransferase reaction of its target protein, eEF2 (eukaryotic elongation factor-2). Currently, this protein-protein interaction is poorly characterized and this study was aimed at identifying the contact sites between eEF2 and the catalytic domain of ETA (PE24H, an ETA from P. aeruginosa, a 24 kDa C-terminal fragment containing a His6 tag). Single-cysteine residues were introduced into the toxin at 21 defined surface-exposed sites and labeled with the fluorophore, IAEDANS [5-(2iodoacetylaminoethylamino)-1-naphthalenesulfonic acid]. Fluorescence quenching studies using acrylamide, and fluorescence lifetime and wavelength emission maxima analyses were conducted in the presence and absence of eEF2. Large changes in the microenvironment of the AEDANS [5-(2-aminoethylamino)-1-naphthalenesulfonic acid] probe after eEF2 binding were not observed as dictated by both fluorescence lifetime and wavelength emission maxima values. This supported the proposed minimal contact model, which suggests that only small, discrete contacts occur between these proteins. As dictated by the bimol. quenching constant (kq) for acrylamide, binding of eEF2 with toxin caused the greatest change in acrylamide accessibility (>50%) when the fluorescence label was near the active site or was located within a known catalytic loop. All mutant proteins showed a decrease in accessibility to acrylamide once eEF2 bound, although the relative change varied for each labeled protein. From these data, a low-resolution model of the toxin-eEF2 complex was constructed based on the minimal contact model with the intention of enhancing our knowledge on the mode of inactivation of the ribosome translocase by the Pseudomonas toxin.

IT **53-84-9**, NAD

RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)

(substrate, binding; eukaryotic elongation factor-2 (eEF2) interaction with ADP-ribosyltransferase domain of Pseudomonas exotoxin A elucidated using site-specific fluorophore labeled exotoxin A mutants)

RN 53-84-9 CAPLUS

CN Adenosine 5'-(trihydrogen diphosphate), P' \rightarrow 5'-ester with 3-(aminocarbonyl)-1- β -D-ribofuranosylpyridinium, inner salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2003:472604 CAPLUS

DOCUMENT NUMBER: 139:49507

TITLE: Synthesis and use of affinity probes directed toward

adenine nucleotide-binding proteins

INVENTOR(S): Campbell, David A.; Wash, Paul

PATENT ASSIGNEE(S): Activx Biosciences, Inc., USA

SOURCE: PCT Int. Appl., 51 pp.

CODEN: PIXXD2

DOCUMENT TYPE: LANGUAGE: Patent English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

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PATENT NO.
                       KIND
                              DATE
                                          APPLICATION NO.
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                       A2
    WO 2003050248
                              20030619
                                          WO 2002-US39073
                                                                20021205
                            20040122
    WO 2003050248
                       A3
        W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
            CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
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            LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
            PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ,
            UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
        RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
            KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
            FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ,
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                              20030717
                                         US 2002-213359
    US 2003134303
                        A1
                                                             P 20011211
PRIORITY APPLN. INFO.:
                                          US 2001-339424P
                                                             A 20020805
                                          US 2002-213359
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AB The invention relates to compns. and methods for the synthesis and use of adenosine nucleotide-binding protein-directed affinity labels. Adenosine nucleotide-binding proteins may be labeled with probes comprising adenosine, or an analog thereof, functionalized at the 5' position with reactive group capable of reacting with an amino acid side chain functionality at an adenosine nucleotide binding site, and at the 2' or 3' position with a tag for sequestering and/or identifying the resulting conjugate. In particular, one such probe is 5'-fluorosulfonylbenzoylamido-2'(3')-(2-TAMRA-amidoethylcarbamoyl)adenosine, shown to effectively label EGF receptor tyrosine kinase in A431 cells and insulin receptor kinase in boiled rat liver lysate. The probes may be used for determining the presence or

amount of one or more adenosine nucleotide-binding proteins in a complex mixture, particularly a cellular mixture, for screening for drugs, and other purposes associated with the presence of the adenine nucleotide-binding protein(s) in a cell or changes in the presence, amount, activity, or relative concentration of the active adenosine nucleotide-binding protein.

IT 446850-58-4P 446850-61-9P 446850-64-2P 446850-79-9P 545400-02-0P 545400-03-1P

RL: BUU (Biological use, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(synthesis and use of affinity probes directed toward adenine nucleotide-binding **proteins**)

RN 446850-58-4 CAPLUS

CN Adenosine, 5'-deoxy-5'-[[4-(fluorosulfonyl)benzoyl]amino]-, 2'(or 3')-[[2-[[3(or 4)-[3,6-bis(dimethylamino)xanthylium-9-yl]-4(or 3)-carboxybenzoyl]amino]ethyl]carbamate], inner salt (9CI) (CA INDEX NAME)

CM 1

CRN 446850-57-3 CMF C17 H17 F N6 O6 S

CRN 446850-52-8 CMF C28 H28 N4 O6 CCI IDS

RN 446850-61-9 CAPLUS

CN Adenosine, 5'-deoxy-5'-[[4-(ethenylsulfonyl)benzoyl]amino]-, 2'(or 3')-[[2-[[3(or 4)-[3,6-bis(dimethylamino)xanthylium-9-yl]-4(or 3)-carboxybenzoyl]amino]ethyl]carbamate], inner salt (9CI) (CA INDEX NAME)

CM 1

CRN 446850-60-8 CMF C19 H20 N6 O6 S

CRN 446850-52-8 CMF C28 H28 N4 O6 CCI IDS

RN 446850-64-2 CAPLUS

CN Adenosine, 5'-deoxy-5'-[(1-oxo-2-propenyl)amino]-, 2'(or 3')-[[2-[[3(or 4)-[3,6-bis(dimethylamino)xanthylium-9-yl]-4(or 3)-carboxybenzoyl]amino]ethyl]carbamate], inner salt (9CI) (CA INDEX NAME)

CM 1

CRN 446850-63-1 CMF C13 H16 N6 O4

446850-52-8 CRN C28 H28 N4 O6 CMF

CCI IDS

446850-79-9 CAPLUS RN

CN Adenosine, $2'(\text{or }3')-[[2-[[3(\text{or }4)-[3,6-\text{bis}(\text{dimethylamino})xanthylium-9-yl]}-$ 4(or 3)-carboxybenzoyl]amino]ethyl]carbamate] 5'-[4-(fluorosulfonyl)benzoate], inner salt (9CI) (CA INDEX NAME)

1 CM

CRN 446850-52-8 C28 H28 N4 O6 CMF

CCI IDS

2 . CM

CRN 57454-44-1 CMF C17 H16 F N5 O7 S

RN 545400-02-0 CAPLUS

CN Adenosine, 5'-[(chloroacetyl)amino]-5'-deoxy-, 2'(or 3')-[[2-[[3(or 4)-[3,6-bis(dimethylamino)xanthylium-9-yl]-4(or 3)-carboxybenzoyl]amino]ethyl]carbamate], inner salt (9CI) (CA INDEX NAME)

CM 1

CRN 545400-01-9 CMF C12 H15 C1 N6 O4

Absolute stereochemistry.

CM 2

CRN 446850-52-8 CMF C28 H28 N4 O6 CCI IDS

RN 545400-03-1 CAPLUS

CN Adenosine, 5'-deoxy-5'-[[4-(fluorosulfonyl)benzoyl]amino]-, 2'(or 3')-[[2-[[3(or 4)-carboxy-4(or 3)-(3,6-diaminoxanthylium-9-yl)benzoyl]amino]ethyl]carbamate], inner salt (9CI) (CA INDEX NAME)

CM 1

CRN 545399-99-3 CMF C24 H20 N4 O6

CCI IDS

CM 2

CRN 446850-57-3 CMF C17 H17 F N6 O6 S

Absolute stereochemistry.

IT 14365-44-7 51600-11-4

RL: RCT (Reactant); RACT (Reactant or reagent)
 (synthesis and use of affinity probes directed toward adenine
 nucleotide-binding proteins)

RN 14365-44-7 CAPLUS

CN Adenosine, 5'-amino-5'-deoxy- (6CI, 8CI, 9CI) (CA INDEX NAME)

RN 51600-11-4 CAPLUS

CN Adenosine, 5'-O-[(4-methoxyphenyl)diphenylmethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 446850-50-6P 446850-53-9P 446850-71-1P

446850-73-3P 446850-76-6P 545400-00-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(synthesis and use of affinity probes directed toward adenine nucleotide-binding proteins)

RN 446850-50-6 CAPLUS

CN Adenosine, 5'-deoxy-5'-[[(1,1-dimethylethoxy)carbonyl]amino]-, 2'(or 3')-[(2-aminoethyl)carbamate] (9CI) (CA INDEX NAME)

CM 1

CRN 446850-49-3 CMF C15 H22 N6 O5

Absolute stereochemistry.

CM 2

CRN 109-58-0

H2N-CH2-CH2-NH-CO2H

RN 446850-53-9 CAPLUS

CN Adenosine, 5'-amino-5'-deoxy-, monoester with 9-[2-carboxy-4(or 5)-[[[2-(carboxyamino)ethyl]amino]carbonyl]phenyl]-3,6-bis(dimethylamino)xanthylium inner salt (9CI) (CA INDEX NAME)

CM 1

CRN 446850-52-8 CMF C28 H28 N4 O6 CCI IDS

CM 2

CRN 14365-44-7 CMF C10 H14 N6 O3

Absolute stereochemistry.

RN 446850-71-1 CAPLUS

CN Adenosine, 5'-O-[(4-methoxyphenyl)diphenylmethyl]-, 2'(or 3')-[(2-aminoethyl)carbamate] (9CI) (CA INDEX NAME)

CM 1

CRN 51600-11-4 CMF C30 H29 N5 O5 Absolute stereochemistry.

CM 2

CRN 109-58-0 CMF C3 H8 N2 O2

 $H_2N-CH_2-CH_2-NH-CO_2H$

RN 446850-73-3 CAPLUS

CN Adenosine, 2'(or 3')-[[2-[[3(or 4)-[3,6-bis(dimethylamino)xanthylium-9-yl]-4(or 3)-carboxybenzoyl]amino]ethyl]carbamate], inner salt (9CI) (CA INDEX NAME)

CM 1

CRN 446850-52-8 CMF C28 H28 N4 O6 CCI IDS

CM 2

CRN 58-61-7 CMF C10 H13 N5 O4

RN 446850-76-6 CAPLUS

CN Adenosine, 2'(or 3')-[[2-[[3(or 4)-[3,6-bis(dimethylamino)xanthylium-9-yl]-4(or 3)-carboxybenzoyl]amino]ethyl]carbamate] 5'-(chloroacetate), inner salt (9CI) (CA INDEX NAME)

CM 1

CRN 446850-75-5 CMF C12 H14 C1 N5 O5

Absolute stereochemistry.

CM 2

CRN 446850-52-8 CMF C28 H28 N4 O6 CCI IDS

RN 545400-00-8 CAPLUS

CN Adenosine, 5'-amino-5'-deoxy-, 2'(or 3')-[[2-[[3(or 4)-carboxy-4(or

3)-(3,6-diaminoxanthylium-9-yl)benzoyl]amino]ethyl]carbamate], inner salt (9CI) (CA INDEX NAME)

CM 1

545399-99-3 CRN CMF C24 H20 N4 O6

CCI IDS

CM 2

CRN 14365-44-7 CMF C10 H14 N6 O3

Absolute stereochemistry.

L13 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

2001:284222 CAPLUS

DOCUMENT NUMBER:

134:307611

TITLE:

Conjugated polymer tag complexes and their

preparation and use in assays

INVENTOR(S):

Leif, Robert C.; Franson, Richard C.; Vallarino, Lidia

PATENT ASSIGNEE(S): USA

SOURCE:

PCT Int. Appl., 104 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.

KIND DATE APPLICATION NO.

DATE

WO 2001027625 WO 2000-US27787 **A1** 20010419 20001007 W: CA, CH, DE, FI, GB, JP, US RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE 20010419 CA 2000-2387380 CA 2387380 AΑ 20001007 EP 2000-968871 EP 1221052 A1 20020710 20001007 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY PRIORITY APPLN. INFO.: US 1999-158718P P 19991008 WO 2000-US27787 W 20001007

Processes are described for: (1) the sequential solid phase synthesis of AB polymers with at least one tag, which can be a light emitting and/or absorbing mol. species (optical-label), a paramagnetic or radioactive label, or a tag that permits the phys. separation of particles including cells. When multiple optical-labels are suitably arranged in three-dimensional space, the energy transfer from one mol. species to another can be maximized and the radiationless loss between members of the same mol. species can be minimized; (2) the coupling of these polymers to biol. active and/or biol. compatible mols. through peripheral pendant substituents having at least one reactive site; and (3) the specific cleavage of the coupled polymer from a solid phase support. The tagged-peptide or polymers produced by these processes and their conjugates with an analyte-binding species, such as a monoclonal antibody or a polynucleotide probe are described. When functionalized europium macrocyclic complexes, as taught in our U.S. patents 5,373,093 and 5,696,240, are bound to polylysine and other peptides, the emitted light increases linearly with the amount of bound macrocyclic complex. Similar linearity will also result for multiple luminescent macrocyclic complexes of other lanthanide ions, such as samarium, terbium, and dysprosium, when they are bound to a polymer or mol.

RN 56-65-5 CAPLUS

CN Adenosine 5'-(tetrahydrogen triphosphate) (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 58-61-7 CAPLUS

CN Adenosine (8CI, 9CI) (CA INDEX NAME)

RN 58-64-0 CAPLUS

CN Adenosine 5'-(trihydrogen diphosphate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 61-19-8 CAPLUS

CN 5'-Adenylic acid (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 85-32-5 CAPLUS

CN 5'-Guanylic acid (8CI, 9CI) (CA INDEX NAME)

RN : 86-01-1 CAPLUS

CN Guanosine 5'-(tetrahydrogen triphosphate) (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 118-00-3 CAPLUS

CN Guanosine (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 146-91-8 CAPLUS

CN Guanosine 5'-(trihydrogen diphosphate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.

2

REFERENCE COUNT:

THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)
SINCE FILE TOTAL
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